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                data from INPADOC
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NEWS 9 MAR 03 MEDLINE file segment of TOXCENTER reloaded
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                 applications.
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     18 APR 28
                Improved searching of U.S. Patent Classifications for
                 U.S. patent records in CA/CAplus
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chain nodes :
7 8 9 11 12 13 14 15 16 17 18 19 23 24 25 26 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
2-9 4-7 5-23 5-32 6-8 11-12 12-13 12-14 15-16 16-17 17-18 17-19 24-25
25-26 25-28 26-29 26-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 4-7 5-6 5-23 5-32 6-8 12-13 12-14
exact bonds :
11-12 15-16 16-17 17-18 17-19 24-25 25-26 25-28 26-29 26-30

G1:0,S

G3:[*1],[*2]

G4:Cy,[*3]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 32:CLASS

L1 STRUCTURE UPLOADED

L1 HAS NO ANSWERS

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=> s 11 sss sam

SAMPLE SEARCH INITIATED 14:50:58 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -100 TO ITERATE

100.0% PROCESSED 100 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS:

PROJECTED ANSWERS:

1401 TO 2599

0 TO

0 SEA SSS SAM L1 L2

=> s 11 sss ful

FULL SEARCH INITIATED 14:51:06 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -2026 TO ITERATE

100.0% PROCESSED 2026 ITERATIONS 12 ANSWERS

161.54

SEARCH TIME: 00.00.01

L3 12 SEA SSS FUL L1

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SINCE FILE TOTAL ENTRY SESSION

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FULL ESTIMATED COST

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L4 19 L3

=> d 14 1-19 bib hitstr

L4 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:902055 CAPLUS

DN 124:105460

TI Competition between two metabolic pathways: oxidation and desulfuration in the thiobarbiturate series

AU Yebga, A.; Menager, S.; Verite, P.; Farnoux, C. Combet; Lafont, O.

CS Lab. pharmacochimie et biopharmacie, Fac. medecine et de pharmacie de Rouen, Saint-Etienne-du-Rouvray, 76803, Fr.

SO European Journal of Medicinal Chemistry (1995), 30(10), 769-77 CODEN: EJMCA5; ISSN: 0223-5234

PB Elsevier

DT Journal

LA English

IT 100317-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in study of oxidation and desulfuration metabolic pathway in thiobarbiturates)

RN 100317-16-6 CAPLUS

CN 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-methylbutyl)-5-(2-propenyl)-2-thioxo-(9CI) (CA INDEX NAME)

S
$$H$$
 O
 $CH_2-CH_2-CHMe_2$

L4 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:93791 CAPLUS

DN 118:93791

TI Prediction and interpretation of some physicochemical and biological properties of a group of barbituric derivatives by the molecular connectivity method

AU Roca, R. M. Soler; March, F. Garcia; Galvez Alvarez, J.; Garcia Domenech, R.

CS Fac. Farm., Univ. Valencia, Valencia, 46010, Spain

SO Anales de Quimica (1992), 88(3), 382-9 CODEN: ANQUEX; ISSN: 1130-2283

DT Journal

LA Spanish

IT 53943-67-2

RL: BIOL (Biological study)

(structure and activity of, mol. connectivity method for prediction of)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

O HN
$$CH_2-CH=CH_2$$
 $CH_2-CH_2-CHMe_2$

L4 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:509089 CAPLUS

DN 113:109089

TI Liquid chromatographic measurement of hydrophobicity constants for N-arylsulfonylglycine aldose reductase inhibitors

AU Clark, C. Randall; Barksdale, Jeffrey M.; Mayfield, Charles A.; Ravis, William R.; DeRuiter, Jack

CS Sch. Pharm., Auburn Univ., Auburn, AL, 36849-5503, USA

SO Journal of Chromatographic Science (1990), 28(2), 83-7 CODEN: JCHSBZ; ISSN: 0021-9665

DT Journal

LA English

IT 53943-67-2

RL: PRP (Properties) (hydrophobicity of, liquid chromatog. measurements in relation to)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

O
$$_{\rm HN}$$
 O $_{\rm CH_2-CH_2-CHMe_2}$

L4 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:485649 CAPLUS

DN 109:85649 ·

TI Hepatic hydroxylation of a barbiturate; competition between the propyl and isoamyl chains

AU Talab, Akram; Lafont, Olivier; Menager, Sabine; Cave, Christian; Miocque, Marcel

CS Lab. Chim. Org., Fac. Pharm., Chatenay-Malabry, 92290, Fr.

SO European Journal of Medicinal Chemistry (1988), 23(1), 25-9 CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA French

OS CASREACT 109:85649

IT 53943-67-2, 5-Allyl-5-(3-methylbutyl)barbituric acid RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

O HN CH₂- CH= CH₂

$$CH_2-CH=CH_2$$

$$CH_2-CH_2-CHMe_2$$

L4 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1982:79447 CAPLUS

DN 96:79447

TI Correlation of reversed-phase capacity factors for barbiturates with biological activities, partition coefficients, and molecular connectivity indexes

AU Wells, Martha J. M.; Clark, C. Randall; Patterson, Richard M.

CS Sch. Pharm., Auburn Univ., Auburn, AL, 36849, USA

SO Journal of Chromatographic Science (1981), 19(11), 573-82 CODEN: JCHSBZ; ISSN: 0021-9665

DT Journal

LA English

IT 53943-67-2

RL: BIOL (Biological study)

(mol. connectivity index and partition coefficient and pharmacol. of, reversed-phase capacity factors correlation with)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{H} & \text{O} \\ \text{HN} & \text{CH}_2\text{--}\text{CH} = \text{CH}_2 \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CHMe}_2 \end{array}$$

L4 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1980:525407 CAPLUS

DN 93:125407

TI Relations between parameters of adsorption chromatography and chemical structure. Part 2. Adsorption energy and biological activity of barbituric acid derivatives

AU Perina, Z.; Sarsunova, M.

CS Res. Inst. Pharm. Biochem., Prague, 130 00, Czech.

SO Pharmazie (1980), 35(3), 146-9 CODEN: PHARAT; ISSN: 0031-7144

DT Journal

LA German

IT 53943-67-2

RL: BIOL (Biological study)
(absorption energy and biol. activity of, partition coefficient and structure in relation to)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & H & O \\
 & HN & CH_2-CH = CH_2 \\
 & CH_2-CH_2-CHMe_2
\end{array}$$

L4ANSWER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN 1976:144562 CAPLUS AN 84:144562 DN TI Molecular connectivity. 6. Examination of the parabolic relationship between molecular connectivity and biological activity Murray, Wallace J.; Kier, Lemont B.; Hall, Lowell H. AU ĊS Massachusetts Coll. Pharm., Boston, MA, USA SO Journal of Medicinal Chemistry (1976), 19(5), 573-8 CODEN: JMCMAR; ISSN: 0022-2623 DTJournal LΑ English IT 53943-67-2 RL: PRP (Properties) (mol. connectivity of, biol. activity in relation to) 53943-67-2 CAPLUS 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) CN

O H O
$$CH_2-CH=CH_2$$
 $CH_2-CH_2-CHMe_2$

L4

(CA INDEX NAME)

1975:601710 CAPLUS AN 83:201710 DN TI Qualitative and quantitative investigation of barbiturate metabolites by GC [gas chromatography]-MS [mass spectrometry] and high-resolution mass spectrometry AU Haskins, N. J.; Lee, M. J.; Millard, B. J. CS Sch. Pharm., London, UK SO Advances in Mass Spectrometry (1974), 6, 181-6 CODEN: AMSPAH; ISSN: 0568-000X DTJournal LΑ English IT 23076-38-2 RL: BIOL (Biological study) (as allobarbitone metabolite) RN 23076-38-2 CAPLUS 5-Pyrimidineacetic acid, hexahydro-2,4,6-trioxo-5-(2-propenyl)- (9CI) (CA CN INDEX NAME)

ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

O HN O
$$CH_2 - CO_2H$$
 $CH_2 - CH = CH_2$

L4ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN AN 1975:478281 CAPLUS 83:78281 DN Intermolecular interaction of some barbituric acid derivatives with TI nitrophenols ΑU Shesterova, A. A.; Petrenko, L. P.; Tzakenaite, A.; Pechenkin, A. G.; Strel'nikova, N. D. Tomsk. Politekh. Inst. im. Kirova, Tomsk, USSR CS SO Izvestiya Tomskogo Politekhnicheskogo Instituta (1974), 198, 97-101 CODEN: ITPKAM; ISSN: 0368-0487 DΤ Journal LA Russian IT 56383-72-3 RL: PRP (Properties)

RN 56383-72-3 CAPLUS
CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-phenyl- (9CI) (CAINDEX NAME)

(complexing of, with p-nitrophenol, uv in relation to)

ANSWER 10 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

L4

AN 1975:15828 CAPLUS DN 82:15828 Carbon-13 NMR spectra of barbituric acid derivatives. II ΤI Okada, Jutaro; Esaki, Toshiyuki AU CS Fac. Pharm. Sci., Kyoto Univ., Kyoto, Japan Chemical & Pharmaceutical Bulletin (1974), 22(7), 1580-7 SO CODEN: CPBTAL; ISSN: 0009-2363 DTJournal LΑ English IT 53943-67-2 RL: PRP (Properties) (carbon-13 nmr of) RN 53943-67-2 CAPLUS 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)-(9CI)(CA INDEX NAME)

$$\begin{array}{c|c} \text{H} & \text{O} \\ \text{HN} & \text{CH}_2\text{--}\text{CH} = \text{CH}_2 \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CHMe}_2 \end{array}$$

L4 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1971:51827 CAPLUS

DN 74:51827

TI Relatioons between chemical structure and pharmacological action in the group of the morpholinoalkyl derivatives of barbiturates and glutethimide substituted at the nitrogen atom

AU Staneva-Stoicheva, Dushka; Petkov, Veselin; Ovcharov, R.

CS Bulg.

SO Farmatsiya (Sofia, Bulgaria) (1970), 20(3), 43-51 CODEN: FMTYA2; ISSN: 0428-0296

DT Journal

LA Bulgarian

IT 31414-80-9

RL: BIOL (Biological study)
(nervous system response to)

RN 31414-80-9 CAPLUS

CN Barbituric acid, 5-allyl-5-isopentyl-1-(2-morpholinoethyl)-2-thio- (8CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{CH}-\text{CH}_2-\text{CH}_2\\ \text{H}_2\text{C}=\text{CH}-\text{CH}_2\end{array} \begin{array}{c} \text{H}\\ \text{N} \\ \text{CH}_2-\text{CH}_2-\text{CH}_2 \end{array}$$

L4 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1970:445445 CAPLUS

DN 73:45445

TI Synthesis and study of acyl derivatives of barbituric acids

AU Kulev, L. P.; Shesterova, A. A.

CS Tomsk. Politekh. Inst., Tomsk, USSR

SO Tr. Nauch. Konf. Tomsk. Otd. Vses. Khim. Obshchest., 1st (1969), 77-9 CODEN: 17VDAE

DT Conference

LA Russian

IT 27890-06-8P

RN 27890-06-8 CAPLUS

CN Barbituric acid, 1-benzoyl-5-isopentyl-5-phenyl- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ Ph - C & & & \\ & & & \\ O & & & \\ \end{array}$$

L4ANSWER 13 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN AN 1969:113522 CAPLUS 70:113522 DN Isolation and identification of brallobarbital metabolites TI ΑU Keding, H.; Schmidt, Georg Inst. Gerichtl. Med., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger. CS SO Arzneimittel-Forschung (1969), 19(3), 342-7 CODEN: ARZNAD; ISSN: 0004-4172 DTJournal German LΑ IT 23076-38-2 RL: BIOL (Biological study) (as brallobarbital metabolite) RN 23076-38-2 CAPLUS

5-Pyrimidineacetic acid, hexahydro-2,4,6-trioxo-5-(2-propenyl)- (9CI)

$$\begin{array}{c|c}
 & H & O \\
 & HN & CH_2 - CO_2H \\
 & CH_2 - CH = CH_2
\end{array}$$

INDEX NAME)

L4ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN ΑN 1964:426765 CAPLUS 61:26765 DN OREF 61:4683f-g Rapid extraction method for barbiturates from blood for gas-liquid chromatographic analysis AU Jain, Naresh C.; Fontan, Charles R.; Kirk, Paul L. CS Univ. of California, Berkeley Microchemical Journal (1964), 8(1), 28-34 SO CODEN: MICJAN; ISSN: 0026-265X DTJournal LΑ Unavailable ΙT 53943-67-2, Barbituric acid, 5-allyl-5-isopentyl-(sodium derivative, determination in blood) RN 53943-67-2 CAPLUS 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)-(9CI)CN (CA INDEX NAME)

$$\begin{array}{c} \text{H} & \text{O} \\ \text{HN} & \text{CH}_2\text{--}\text{CH} = \text{CH}_2 \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CHMe}_2 \end{array}$$

L4 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:39327 CAPLUS

DN 58:39327

OREF 58:6646c-d

TI Determination of barbituric acid derivatives with tetramethylammonium hydroxide in anhydrous media

AU Rink, Melanie; Riemhofer, Monika

CS Univ. Bonn, Germany

SO Deutsche Apotheker Zeitung (1962), 102, 1567-71 CODEN: DAZEA2; ISSN: 0011-9857

DT Journal

LA Unavailable

IT 53943-67-2, Barbituric acid, 5-allyl-5-isopentyl-(determination of, tetramethylammonium hydroxide in)

RN 53943-67-2 CAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methylbutyl)-5-(2-propenyl)- (9CI) (CA INDEX NAME)

O HN
$$CH_2-CH=CH_2$$
 $CH_2-CH_2-CHMe_2$

L4 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1960:23154 CAPLUS

DN 54:23154

OREF 54:4598a-e

TI The ultraviolet absorption spectra and the dissociation constants of the derivatives of thiobarbituric acid

AU Sato, Yoshishige

CS Tanabe Pharm. Co. Ltd., Osaka

SO Nippon Kagaku Zasshi (1957), 78, 921-3 CODEN: NPKZAZ; ISSN: 0369-5387

DT Journal

LA Unavailable

IT 100317-16-6, Barbituric acid, 5-allyl-5-isopentyl-2-thio-(phys. properties of)

RN 100317-16-6 CAPLUS

CN 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-methylbutyl)-5-(2-propenyl)-2thioxo-(9CI) (CA INDEX NAME)

S
H
N
$$CH_2-CH=CH_2$$
 $CH_2-CH_2-CHMe_2$

L4 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1958:45654 CAPLUS

DN 52:45654

OREF 52:8214d-i,8215a-c

TI Barbituric acid derivatives

IN Scheffler, Heinz; Kottler, August

PA C. H. Boehringer Sohn

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI US 2820035 19580114 US

RN 817637-73-3 CAPLUS

CN Barbituric acid, 5-isopentyl-5-(5-norbornen-2-yl)- (6CI) (CA INDEX NAME)

L4 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1958:11436 CAPLUS

DN 52:11436

OREF 52:2095d-g

TI Barbituric acid derivatives

PA Dr. Karl Thomae G. m. b. H. Chemisch-pharmazeutische Fabrik.

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI GB 777813 19570626 GB

RN 817637-73-3 CAPLUS

CN Barbituric acid, 5-isopentyl-5-(5-norbornen-2-yl)- (6CI) (CA INDEX NAME)

L4 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1954:71567 CAPLUS

DN 48:71567

OREF 48:12677c-g

TI Barbituric acids

AU Moffett, Robert B.; Stafford, James E.; Hart, Charlotte A.

CS Sterling-Winthrop Research Inst., Rennselaer, NY

SO Journal of the American Pharmaceutical Association (1912-1977) (1953), 42, 720-1

CODEN: JPHAA3; ISSN: 0003-0465

DT. Journal

LA Unavailable

IT 669091-73-0, Barbituric acid, 5-cyclopentyl-5-isopentyl-842952-67-4, Barbituric acid, 5-(2-cyclopenten-1-yl)-5-isopentyl-

(preparation of)

RN 669091-73-0 CAPLUS

CN Barbituric acid, 5-cyclopentyl-5-isopentyl- (5CI) (CA INDEX NAME)

RN 842952-67-4 CAPLUS

CN Barbituric acid, 5-(2-cyclopenten-1-yl)-5-isopentyl- (5CI) (CA INDEX NAME)

=> log y
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

10/763,904

FULL ESTIMATED COST

64.86 226.40

STN INTERNATIONAL LOGOFF AT 14:51:38 ON 03 MAY 2005